

MODAC

Version 1

A Hydrogeology-Based Parameter Estimation Program for Groundwater Flow Model

Developed
by

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INTRODUCTION

This document serves as the user's manual of MODAC, a hydrogeology-based parameter estimation package for groundwater flow model calibration.

1.1 What is MODAC

MODAC is a parameter estimation package for groundwater flow model calibration. It couples the widely used three-dimensional groundwater flow model MODFLOW (1996 version) and the inverse hydraulic parameter estimation procedures developed by Guo and Zhang (1994, 2000).

MODAC is an indirect inverse solution procedure. The numerical procedure is an iterative process that performs MODFLOW simulation and parameter adjustment alternatively. It starts from a set of initial estimates of hydraulic parameters, and improves the estimates according to the derived optimality condition (Appendix A). The iterative process gradually reduces the differences between the simulated and interpreted hydraulic gradient and hydraulic head as well as between the simulated and estimated boundary fluxes.

MODAC has been used for extensive applications on various real-world groundwater model calibrations. Results of these applications have demonstrated that MODAC can significantly improve quality and efficiency of model calibration.

1.2 Role of MODAC in Model Calibration

Groundwater model calibration involves estimation of hydraulic parameters and hydrology parameters, and verification of conceptual model. The hydraulic parameters hereafter refer to the parameters that reflect the hydraulic characteristics of a groundwater flow system. They include hydraulic conductivity, transmissivity, head-dependent boundary conductance, vertical conductance, and storage coefficient or specific yields. Hydrologic parameters hereafter refer to sink and source, such as groundwater recharge, evaporation, and extraction or injection rates. The current version of MODAC only automatically estimates hydraulic parameters under steady state conditions, including

- Hydraulic conductivity (transmissivity)
- Head-dependent boundary conductance
- Vertical conductance

The hydrologic parameters (sink and source) need to be estimated independently prior to model calibration and to be adjusted during iterative model calibration processes.

1.3 Features of MODAC

MODAC is a hydrology-based parameter estimation package. The concept that guides parameter adjustment is consistent with Darcy's law (Appendix A), which, in essence, is

different from those parameter estimation packages based on non-linear regression method. The general features of MODAC are listed as follows and explained in detail in the main text:

- MODAC is specifically developed for groundwater flow model calibration, thus only applicable to groundwater flow model.
- Effective use of MODAC for model calibration requires rigorous conceptual model development with a global calibration target and to be implemented with an iterative calibration procedure.
- Interpreted groundwater potentiometric surface based on measured hydraulic heads is used as direct calibration target.
- Estimated or measured fluxes are used as secondary calibration target.
- Constraints on hydraulic conductivity and conductance are directly applied in parameter estimation process.
- No zonation of parameters is required; parameter adjustment is performed based on cell-by-cell basis.
- Smoothing technique is used to minimize spatial variation of parameter.
- The current version of MODAC is only for steady state condition. Transient condition will be included in the later version.

1.4 Why Use MODAC

- Calibration results not only match observed heads at measurement points but also match hydraulic gradients, general flow pattern, flow paths, and measured (estimated) fluxes.
- Computation time is significantly less than the time required by nonlinear least squares methods, because multiple-optimization problem is solved by many one-dimensional problems simultaneously (Appendix A).
- Particularly powerful and efficient in calibrating highly heterogeneous aquifer and matching large quantity of observations with small residuals. The more the data, the more the confident of calibration.
- No limit on number of hydraulic parameters to be estimated, thus highly heterogeneous aquifer can be easily calibrated.
- Calibration procedure does not cause dry cell problem attributable to numerical isolation.
- Easy to understand, easy to use, and easy to identify problems associated with conceptual model.

1.5 Installation and Uninstallation of MODAC

If you have old version of MODAC, please uninstall the package following the instruction under Uninstallation first.

Installation

Installation of MODAC is similar to other Windows products as following steps:

- Unzip the MODAC package in a separate folder
- Click *setup.exe*, installation will automatically start

If this is the first time to install MODAC, you may see a note, “This is a demo version, results cannot be saved.” This means that without registration to get a security code, you may try the examples or play with your cases, but you will not be able to save the results.

Uninstallation

Uninstallation of MODAC is similar to other Windows program as following steps:

- Double-click *My Computer* in the upper left corner of the desktop
- Double-click *Control Panel* and then double-click the *Add/Remove Programs* icon
- Select MODAC from the list of programs and click the *Add/Remove* button on the dialog

Then follow the prompts from the uninstall wizard from there.

1.6 Obtaining a Security Code

MODAC package is protected by a security code that is tied with your computer. If you want to obtain a standard version, you must obtain a security code to complete installation. To obtain a security code, please do the following:

- Go to **File** and select **Register**
- A code registration dialog displays the **System Code**. Copy the **System Code**, then send it via an email to Chuan-Mian_Zhang@urscorp.com, including your name, affiliation, and email address. You will get an email back and receive a **Security Code**. If you obtain the code from Groundwater Vistas, please send the information to support@groundwatermodels.com.
- Enter this **Security Code**, then click **Register**, your are registered and complete the installation

If the security code is invalid or expired, MODAC will run as a demo version, no results can be saved.

1.7 Technical Support

For questions, you may send an email to Chuan-Mian_Zhang@urscorp.com

1.8 How to Use This Manual

This manual describes the general concept of MODAC and detailed instruction of how to use MODAC. Section 2 discusses the concept of using MODAC in model calibration. Section 3 provides a tutorial for first-time users with demonstration of hypothetical cases. Section 4 includes descriptions of data preparation and input instruction. Appendixes include theoretical background for the inverse method, numerical procedures, and discussion for hypothetical case. Electronic files for three hypothetical cases are included for users to understand how MODAC works and how to use MODAC.

2 CONCEPT OF MODAC TO SUPPORT GROUNDWATER FLOW MODEL CALIBRATION

A groundwater flow model development involves understanding of site hydrogeology, conceptual model development, conversion of conceptual model to appropriate numerical model design, estimation of hydrologic and hydraulic parameters, and evaluation of calibration results comparing to observations. The last two steps are often referred to as model calibration. Model calibration is the most important and perhaps the most difficult part of a groundwater flow model development. Quality of model predictions is highly dependent on the quality of model calibrations.

To date, there is no standard protocol for groundwater flow model calibration, because site conditions and modeling objectives are highly variable. Level of calibration and process of calibration often depend on modeling objectives and data availability. Here we present our understanding about concept of model calibration and propose a process of performing model calibration using MODAC.

We often have two concerns regarding to model calibration:

- Should calibration be performed for hydraulic parameters (e.g., hydraulic conductivity) and stresses (e.g., pumping rate, groundwater recharge) at the same time?
- Should calibration results be only compared to spot-wise measurements, or also compared to overall flow pattern?

The discussions in the following text present our understanding about the above concerns, focusing on:

- Calibration of hydraulic parameters versus stresses
- Targets of model calibration

2.1 Calibration of Hydraulic Parameters versus Stresses

Ideally, model calibration is to perform a quantitative *physical characterization* for an aquifer or a groundwater flow system, given known *stresses* and observed aquifer *responses*. The physical characteristics of an aquifer usually comprise of:

- Dimension and geometry of hydrogeologic units
- Hydraulic conductivity (or transmissivity) distributions
- Types of boundary conditions and related hydraulic conductance
- Storage coefficient or specific yield

The physical characteristics of a groundwater flow system are usually measured in field at discrete points by geologic borings and aquifer tests, and then interpreted qualitatively through conceptual model development.

Among the physical characteristics, the dimension and geometry of hydrogeologic units are often represented by model configuration, including layers, thickness, and bottom elevations. These are considered as numerical model structure, which are designed prior to parameter adjustment and are usually not to be changed unless it is necessary. The type of boundary conditions is also specified prior to parameter estimation. The other three items, i.e., hydraulic conductivity (or transmissivity), head-dependent boundary conductance, and storage coefficient, are conventionally considered as hydraulic parameters. They need to be intensively adjusted during model calibration. This hydraulic parameter estimation process is often referred to as the inverse process in the inverse technique literature.

Stresses usually are referred to as groundwater recharge, evapotranspiration, and source/sink, which are placed at the right-hand-side of a groundwater governing equation. Aquifer responses are usually referred to as groundwater hydraulic heads and fluxes. Both stresses and responses can vary over time, while the physical characteristics of a groundwater flow system are inherent and supposed not to change over time under normal conditions (in an average field scale sense).

Model calibration refers to a process that estimates the physical characteristics of a groundwater flow system given stresses and responses, while model prediction refers to a process that estimates aquifer responses given a calibrated flow system and potential stresses. If the physical characteristics are calibrated well, the prediction results should be representative when stresses to a groundwater system are changed.

The calibration process described above is an ideal process that may only be found in a laboratory or in a hypothetical case. In real-world modeling, a lot of information is only known at sparsely distributed points or known with some uncertainty, including both hydraulic parameters and stresses. Therefore, model calibration has to deal with estimation of both hydraulic parameters and stresses. However, because hydraulic parameters and stresses are highly correlated in a model calibration, MODAC does not deal with them at the same time.

Facing the practical complexity, we propose to *decompose* the model calibration process into separate steps, and then integrate these steps together through an *iterative* process. Hydraulic parameter estimation and stress estimation can be decomposed into separate steps using different approaches. Stresses can be estimated independently prior to groundwater model calibration. Groundwater recharge can be estimated using various hydrology methods, and source/sink can be estimated based on field investigations, water use records, and water budget analysis. Based on the independently estimated stresses, hydraulic parameters can be estimated using the groundwater flow model inverse procedures, such as MODAC. In this way, we could sufficiently use as much information as possible. Uncertainty related to correlation of hydraulic parameters and stresses can be controlled to a relatively low level.

In a groundwater flow model calibration the role of MODAC (version 1) is only to automatically estimate aquifer hydraulic parameters. This is only one of the components

of a complete model calibration. However, it is usually the most time-consuming and most difficult task in a model calibration. MODAC can significantly speed up this process and to improve model calibration result.

2.2 Targets for Model Calibration

Targets for model calibration are those available aquifer responses including measured hydraulic heads or fluxes. It is common that a model calibration is only evaluated by comparing simulated hydraulic head to measured head at sparsely distributed points using statistics. Based on our practical modeling experiences, it is important to have a global calibration target for model calibration. A global target includes not only point-wise measured heads but an entire flow pattern, hydraulic gradient, flow pathways, fluxes, seep locations and flow rates, water budget, and field aquifer test results, as well as groundwater contaminant migration information, if it is relevant.

To meet such a global calibration target, we propose to include an interpreted potentiometric surface map as one of the calibration targets. A representative potentiometric surface will include flow pattern, hydraulic gradient, and flow pathways. It is a common practice for a site hydrogeologic characterization to prepare a groundwater potentiometric surface, which should be interpreted based on measured hydraulic heads and understanding of hydrogeologic conditions.

Using potentiometric surface as a calibration target is a special requirement using MODAC. Advantages of using potentiometric surface as one of calibration targets are:

- From a conceptual model development point of view, a potentiometric surface is a key component of conceptual model development, which contains qualitative and quantitative geologic and hydrogeologic information, including flow directions, hydraulic gradient, and flow path, which may not be fully reflected from only point-wise head measurements.
- Based on Darcy's law, a steady state potentiometric surface may reflect a subsurface hydraulic parameter distribution pattern, or an equivalent subsurface hydraulic parameter distribution pattern. Thus preconceived zonation for parameter structure may not be necessary.
- From a numerical point of view, a potentiometric surface provides measured or estimated hydraulic heads for all model cells, which mitigates the so-called ill-posed problem in inverse technology.
- The process of matching the potentiometric surface in a model calibration would warrant matching calculated hydraulic heads with measured hydraulic heads at well locations, if the interpretation of potentiometric surface honor observations.
- Using an interpreted potentiometric surface as calibration target will avoid dry cell problems that are attributable to numerical isolation, which is a commonly accounted problem in the inverse procedure using non-linear least squares methods.

It should be noted that, targets of model calibration using MODAC are not limited to potentiometric surface. Application of MODAC in model calibration requires using a global target, which should include all the following components if it is possible:

- Potentiometric surface and measured hydraulic heads
- Measured or estimated fluxes
- Water budget analyses
- Field aquifer test results
- Groundwater contaminant migration direction, pathways, and velocity

Meeting such a comprehensive global calibration target can only be accomplished through an iterative calibration process that comprise of several decomposed steps as mentioned in Section 2.1.

3 TUTORIAL WITH HYPOTHETICAL CASE DEMONSTRATION

This section illustrates how MODAC works through demonstration using hypothetical cases.

3.1 Running MODAC with Hypothetical Case 1

Hypothetical Case 1 assumes an unconfined and heterogeneous groundwater flow system. The specified hydraulic conductivity distribution ranges from 0.1 ft/day to 10.0 ft/day. The bottom elevation of the aquifer is variable. A one-layer, finite difference grid consisting of 100 rows and 100 columns with a uniform cell dimension of 100 ft by 100 ft is superimposed on the flow system. Boundary conditions consist of general head boundary, prescribed flux, and no-flow. The conductance of the general head boundary is constant and specified as 250 ft²/day. Several source/sink terms exist within the model domain, including two pumping wells, two injection wells, and areal positive and negative ground water recharge. The hydraulic head distribution was generated using MODFLOW input file data under steady-state condition.

In the parameter estimation process, the hydraulic conductivity distribution and general head boundary conductance are assumed unknown. The generated hydraulic head distribution is assumed to be the “interpreted” potentiometric surface and is used as the calibration target for parameter estimation. In total, 10,000 hydraulic conductivity values and 100 conductance values need to be estimated given 10,000 known hydraulic head values, specified boundary conditions, and other parameters.

Parameter estimation is an iterative forward process, which follows the numerical procedure as described in Appendix A. The initial hydraulic conductivity distribution is assumed to be constant over the entire model domain. The upper limit and lower limit on hydraulic conductivity is set as constant as 100 ft/day and 0.001 ft/day, respectively.

To run MODAC on Case 1, please follow the steps below.

- 1) Unzip Case1.zip in a new folder, you will see standard MODFLOW files with root name as Case1
- 2) Click MODAC icon to start the program
- 3) Go to **File** and click **NEW ... (MODFLOW NAM file)**, browse for Case1.nam
- 4) Go to **Setup** and click *Import MAC file*, then import file Initial.mac. After reviewing the content of the MAC file, click *Save MAC*. You may review the initial setup of Case 1 under **Graphic**, including bottom elevation, water table, thickness, hydraulic conductivity, upper limits on hydraulic conductivity, and lower limits on hydraulic conductivity
- 5) Go to **File** again, click **Open ... (MODAC NFL file)** – browse for Case1.nfl
- 6) Go to **Run**, you will see Model Run Dialog

Model Run Dialog

Number of Calibration Step
50

Selecting Method

Primary Method	Secondary Method	Alternating Interval
Combined Head Gradient	Combined Head Gradient	2

Selecting Parameter for Calibration

- ☒ Hydraulic Conductivity or Transmissivity
- ☒ General Head Conductance
- ☐ Drain Conductance
- ☐ River Conductance
- ☐ Storage Coefficient

☐ Zone Average ☒ Smooth

Vertical Conductance

Smooth Factor

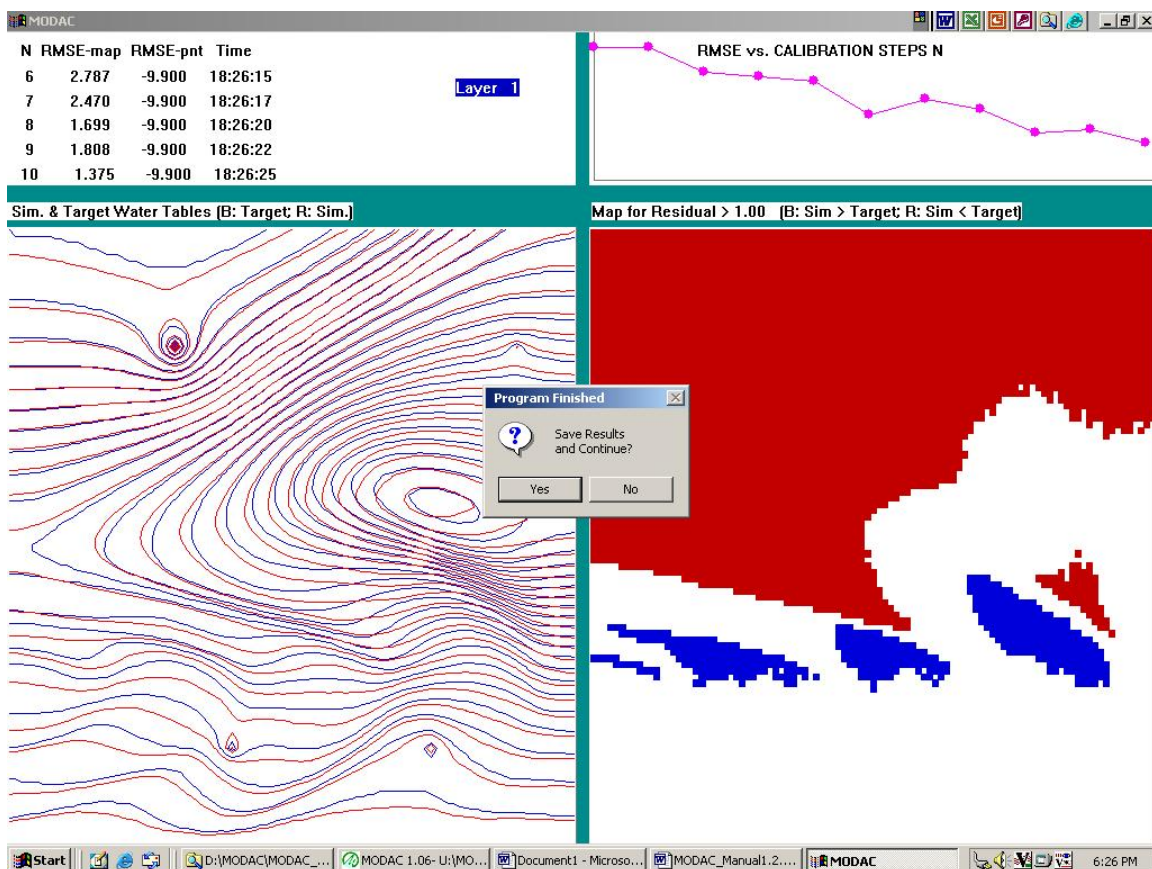
- ☒ Uniform for all layer
- Upper Ratio (≥ 1.0) 1.15
- Lower Ratio (≤ 1.0) 0.6

Maximum MODFLOW Iteration 5

OK Cancel

7) In Model Run Dialog,

- Set *Number of calibration* step = 50
- Check *Smooth*
- Set *Maximum MODFLOW iteration* = 5 (for Case 1, it is the PCG external iteration number)
- Click *OK*. You will see the target potentiometric surface first, and then four windows on screen



TOP-LEFT WINDOW

N RMSE-map RMSE_pnt Time Layer

Where

N	Number of calibration steps
RMSE-map	Root-mean-squared error between simulated and target head values over entire model domain of the layer
RMSE-pnt	Root-mean-squared error between simulated and observed head values at measurement points
Time	Operation time
Layer	Layer number

During MODAC operation, you should see the RMSE-map is progressively decreasing with time if the program works well. In Case1, observed values are not inputted, thus, RMSE-pnt is a default value of -9.900.

TOP-RIGHT WINDOW

A dynamic curve of RMSE vs. calibration steps is displayed to show the trend of root-mean-squared error, which is consistent with what is displayed in the top-left window. If

the curve moves down, the parameter estimation works well and towards convergence. If the curve moves up, the parameter estimation is having difficulty, either the internal constraints (e.g., upper or lower limit of hydraulic conductivity) have been exhausted, or the estimation is being locked or bounded in local areas. In these cases, you may need to try different methods as primary method or secondary method, and/or choose different alternating interval number. You may also turn on or turn off **Smooth** to either limit the spatial variation or do not limit the spatial variation during parameter estimation. When the curve approaches flat (i.e., no improvement in matching the gradient or head), and if the RMSE is acceptable, you may accept the estimation results and save the results. If the RMSE is still pretty large, you may try to adjust the methods and the smooth factors. If all these adjustments do not help, you may go back to check your model setup and conceptual model.

BOTTOM-LEFT WINDOW

This window shows comparison of target and calculated potentiometric surfaces at every calibration step. Target potentiometric surface is in blue and does not change with iterations. Calculated potentiometric surface is in red and changes with iterations. If MODAC works smoothly, red contour lines should gradually match blue contour lines.

BOTTOM-RIGHT WINDOW

This window displays residual map showing residuals between target head and simulated head at every calibration step. Blue color indicates calculated head is higher than target head, and red color means calculated head is lower than target head. If both blue and red color spots reduce with time, parameter estimation is working well. Ideally all color zones should disappear gradually, implying all the residuals are below a predefined residual value (head residual criteria for screen plot). If color spots in certain area persist, you may need to either adjust the methods, or go back to original model to check the conceptual model and numerical model setup.

Screen plot of residual zone depends on selected criteria (i.e. predefined residual value) for plotting. The criteria can vary depending on your problem. A default value for residual plotting criteria is 1.0 feet.

When MODAC finishes the run, select *Save Result* to continue, you will be back to Model Run Dialog.

8) In Model Run Dialog,

- Set *Number of calibration step* = 10 or more
- Increase *Maximum MODFLOW iteration* = 40 to let solution converge

After repeating step 7 for a few times, you should see match of the simulated and target water tables reasonably well in the bottom-left window, and residuals in bottom-right window disappearing.

9) Review Results

You may review the results under **Graphic** after run or at any time, or import the results to any groundwater model graphic-user-interface (GUI). The true hydraulic conductivity distribution of Case 1 is provided in Appendix B. The calibrated one should be fairly close to the true distribution. Be sure to check water budget for the final results. However, in the early stage of parameter adjustment, as long as the solution is not isolating, fewer iteration steps can be used to speed up the process and the early results do not have to meet the converge discrepancy criteria. The decision is often problem specific and depending on experiences.

3.2 Running MODAC with Hypothetical Case 2

Hypothetical Case 2 is a three-layer model case. The three model layers are assumed hydraulically connected. The hydraulic conductivity values range between 0.005 ft/day to 50 ft/day. A river running through the center of the model domain is one of the main groundwater discharge zone. The primary source of water to the groundwater flow system is areal groundwater recharge. The external boundary conditions include prescribed head, general head, and no-flow boundaries. Similar to Case 1, the MODFLOW simulated hydraulic head distributions are assumed as the target potentiometric surface for hydraulic parameter estimation, while the hydraulic conductivity distribution, the river conductance, and the conductance for the general head boundary are assumed unknown.

Case 2 is illustrated through two conditions:

- Case 2 - Potentiometric surfaces are used as calibration target, while boundary fluxes are evaluated and adjusted by users externally. This is usually the case when you just start a model calibration and do not have a good sense about boundary fluxes.
- Case 2 plus - Both potentiometric surfaces and estimated boundary fluxes are used as calibration targets (Section 3.4)

To run MODAC on Case 2, you have two choices for parameter estimation. One is to assume the target potentiometric surface is known for all the three layers. The other choice is to assume that the target potentiometric surface is only available for first layer. The second choice is fairly common in actual conditions. Let us introduce the first choice now and you may try second choice by yourself. Please follow the steps below.

- 1) Unzip Case2.zip in a new folder
- 2) Click MODAC icon to start the program

- 3) Go to **File** and click **NEW ... (MODFLOW NAM file)**, browse for Case2.nam
- 4) Go to **Setup** and click *Import MAC file*, then import Initial.mac. You will see a MODAC MAC Setup window as follow:

You may review the MODAC MAC setup window and click *Save MAC*.

- 5) Go to **File** again, click **Open ... (MODAC NFL file)** – browse for Case2.nfl. You may review the setup under **Graphic**, including initial hydraulic conductivity, upper and lower limits on hydraulic conductivity. You will see the upper limits on hydraulic conductivity of layer 1 is distributed while the constraints for others are constant.
- 6) Go to **Run**, in Run Dialog,
 - Set *Number of calibration step* = 100
 - Check *Smooth*

- Select *Calculate leakance*
- Set *Maximum MODFLOW iteration* = 5 (for Case 2, it is the PCG external iteration number)
- Click *OK* and let MODAC to run

You will see each window is updating three times for each calibration step, following a sequence of Layer 3, Layer 2, and Layer 1. In the top-left window, the RMSE-pnt value is also changing with time, because a file with observed head values is placed in the same directory with a name of target.dat, thus comparison between simulated head and observed head is available.

In the bottom-left window, you will also see that Layer 1 is dry in some areas in the early calibration steps. However, the dry area gradually reduces and disappears with increased calibration steps. This is because that the target water levels are higher than the bottom elevation, not dry; and the parameter adjustment is working toward the direction to make the simulated water levels match the

target levels. Thus, when you see such initial dry conditions, do not turn on the “rewetting” function in MODFLOW, just let MODAC work.

When MODAC operation is done, select *Save Result* to continue, you will be back to Run Dialog.

- 7) In Run Dialog,
 - Set *Number of calibration step* = 10 or more
 - Increase *Maximum MODFLOW Iteration* = 100 to let solution convergeRepeat step 7 as many times as you like until you satisfy your results.
- 8) Import the results into a (GUI) to review water budgets and calibration statistics. Most of MODAC files, such as K, Vcont, and upper and lower limits for K, can be conveniently reviewed or modified under **Graphic** in MODAC or exchanged with GV as matrix files. You can review or modify them either in GUI or in MODAC.

3.3 Model Run Dialog Instruction

Number of Calibration Step

Each calibration step includes a MODFLOW simulation and a MODAC parameter adjustment. When you start a problem, you may try a small number first, like 5 to 20. No limit on number of calibration steps.

Alternating Interval

Alternating interval is the number of steps using primary method. If alternating interval equals 1, adjustment will use one step of primary method and one step of secondary method. If alternating interval is equal to or greater than 2, adjustment will use two or more steps of primary method and one step of secondary method.

Selecting Parameter for Calibration

The parameters that you can use MODAC to estimate include:

- **Hydraulic conductivity**
- **General head conductance**
- **River conductance**
- **Drain conductance**
- Storage coefficient (not applicable yet)

Zone Average

If clicking this button, the distributed K within a specified zone will be averaged. You may click this button after your calibration results are generally acceptable, depending on your need.

Smooth

Smooth technique should be applied during parameter estimation. It tends to minimize spatial variation of parameter values when MODAC tends to vary parameter values to meet the optimality conditions. Therefore, smooth technique plays a role to overcome potential over-parameterization.

However, sometimes smoothing could limit variation of parameters at a local area, which would limit continuation of parameter estimation. In this case, you may turn off the smooth function, let MODAC to work in a more flexible environment. If the results are improved, you may turn on the smooth factor again.

When you click *Smooth*, in Run Dialog, you may specify the upper ratio and lower ratio. You can change these ratios any time during MODAC operation.

Vertical Conductance

You have three options depending on need and data availability:

- **Keep leakance**
- **Calibrate leakance**
- **Calculate leakance**

Keep leakance - Vertical conductance will not change during parameter adjustment. This is used only for limited conditions.

Calibrate leakance - Vertical conductance will be calibrated based on comparison of vertical hydraulic gradient between layers. This is only used when representative potentiometric surfaces are available for both upper and lower layers.

Calculate leakance - Vertical conductance will be calculated at every calibration step according to estimated hydraulic conductivity with specified vertical anisotropy ratios. This is a commonly used option.

Maximum MODFLOW Iteration

The maximum MODFLOW iteration here refers to the number of MODFLOW solver iterations. The MODFLOW solver package requires specification of maximum calculation iterations. In MODAC operation, as long as your MODFLOW solution is stable, in early stage of parameter adjustment, you may chose a number that is smaller than the number of iteration specified in the MODFLOW solver package to speed up the parameter estimation process. Please be cautious when selecting the maximum MODFLOW iteration. For final results, you must select a proper number of iteration to meet a predetermined converge criteria.

3.4 Running MODAC with Hypothetical Case 2 Plus

As an important model calibration target, boundary fluxes should be introduced during parameter estimation process. MODAC provides you opportunities to specify a range of estimated fluxes as a secondary calibration target. During the process, MODAC tries to adjust parameters so that the calculated fluxes to stay within the specified range or to approach the specified range.

You may specify lower limit and upper limit for one type of boundary condition by

- Either total inflow flux or total outflow flux (but not the net of both fluxes)
- Distributed fluxes at boundary cells

depending on your need.

Let us illustrate Case 2 plus by following the steps below.

- 1) Unzip Case2flx.zip in a new folder
- 2) Click MODAC icon to start the program
- 3) Go to **File** and click **NEW ... (MODFLOW NAM file)**, browse for Case2flx.nam
- 4) Go to **Setup** and **Boundary Constraints**, you will see options as
 - GHB
 - River
 - Drain
 - Constant head (CHD)

The image shows a dialog box titled "RIV" with a close button (X) in the top right corner. The dialog is divided into two main sections: "Total Flux Control" and "Individual Cell Limits".

Total Flux Control:

- Two radio buttons are present:
 - ☒ Constrain Total Flux from Aquifer to Boundary (Flux Out)
 - ☐ Constrain Total Flux from Boundary to Aquifer (Flux In)
- Below the radio buttons are two text input fields:
 - "Upper Limits of Total Flux In or Out" with the value "-8.50E+04".
 - "Lower Limits of Total Flux In or Out" with the value "-7.80E+04".

Individual Cell Limits:

- A "File:" label followed by a text input field and a "Browse..." button.
- Four rows of settings, each with a label and a text input field:
 - "Column No. for Lower Limits of Conductance" with the value "7".
 - "Column No. for Upper Limits of Conductance" with the value "8".
 - "Column No. for Lower Limits of Flux" with the value "9".
 - "Column No. for Upper Limits of Flux" with the value "10".

On the right side of the dialog, there are two buttons: "Save" and "Cancel".

Click one of these boundary conditions you will see a dialog window for each of the boundary fluxes as above.

The upper portion of the window is used to specify total fluxes and the lower portion for distributed fluxes. Negative value means fluxes out of an aquifer and positive value means fluxes into an aquifer.

For Case2flx, we specified the ranges of distributed fluxes for the river cells and the ranges of total fluxes for GHB, River, and CHD. We have prepared a .csv file (Riverflx.csv) for distributed range for river fluxes for every river cell. You may browse this file by clicking browse in the lower portion of the dialog window. Note, the specified lower and upper limit for each river cell was assumed with a wider range, because lack of specific information. However this provides you an example so that when you need and have data you may specify the range for certain section. For the sections where you do not have data, you may simply specify a broad range as dummy ranges. The river input file may be prepared in the form of .csv file by Microsoft Excel. As the result of browse, you will see a dialog window as follows.

RIV

Total Flux Control

☒ Constrain Total Flux from Aquifer to Boundary (Flux Out)

☐ Constrain Total Flux from Boundary to Aquifer (Flux In)

Upper Limits of Total Flux In or Out: -8.50E+04

Lower Limits of Total Flux In or Out: -7.80E+04

Save

Cancel

Individual Cell Limits

File: D:\MODAC\MODAC_CASES\Cas2flx

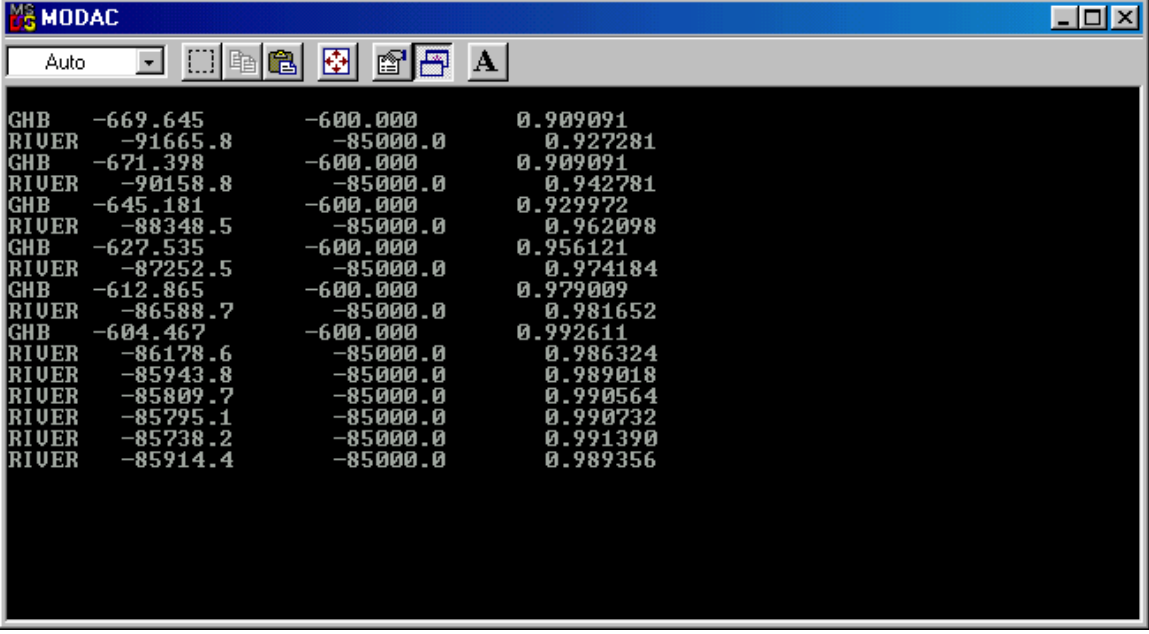
Column No. for Lower Limits of Conductance: 7

Column No. for Upper Limits of Conductance: 8

Column No. for Lower Limits of Flux: 9

Column No. for Upper Limits of Flux: 10

- 5) Go to **File** and chose **Save**. Then chose **Open ... (MODAC NFL file)** and browse for Case2flx.nfl.
- 6) Go to **Run**, and specify a few number of runs and specify other parameters accordingly. This time you will see a DOS window as follows:



The screenshot shows a DOS-style window titled "MODAC". The window contains a table with four columns: Boundary Type, Calculated Flux, Specified Value, and Coefficient. The table lists data for GHB and RIVER boundaries across 16 rows. The first column alternates between "GHB" and "RIVER". The second column shows calculated flux values, the third column shows specified values (mostly -600.000 or -85000.0), and the fourth column shows coefficients. The window has a menu bar with "Auto" and a toolbar with various icons.

Boundary Type	Calculated Flux	Specified Value	Coefficient
GHB	-669.645	-600.000	0.909091
RIVER	-91665.8	-85000.0	0.927281
GHB	-671.398	-600.000	0.909091
RIVER	-90158.8	-85000.0	0.942781
GHB	-645.181	-600.000	0.929972
RIVER	-88348.5	-85000.0	0.962098
GHB	-627.535	-600.000	0.956121
RIVER	-87252.5	-85000.0	0.974184
GHB	-612.865	-600.000	0.979009
RIVER	-86588.7	-85000.0	0.981652
GHB	-604.467	-600.000	0.992611
RIVER	-86178.6	-85000.0	0.986324
RIVER	-85943.8	-85000.0	0.989018
RIVER	-85809.7	-85000.0	0.990564
RIVER	-85795.1	-85000.0	0.990732
RIVER	-85738.2	-85000.0	0.991390
RIVER	-85914.4	-85000.0	0.989356

Four columns are shown in this window. The first column is the type of boundary. In this window, only GHB and River are present. This means that the calculated flux for CHD is already in the range. The second column is the calculated flux at the corresponding calibration step. The third column is the specified value for either lower limit or upper limit. The fourth column is the coefficient calculated by MODAC to adjust the corresponding boundary flux. In this window, the calculated GHB flux is -669.645 initially, which is greater than the specified upper limit, so the corresponding coefficient is 0.909091. In line 9, the GHB flux drops to -604.467, which is close to the specified value of -600.000. After that, GHB disappears, indicating the calculated GHB flux is within the range of specification. The River flux initially -91665.8, which is much greater than the specified upper limit of -85000.0, thus the corresponding coefficient is always less than 1.0. By iteration of 10, or last line in the window, the River flux drops to -85914.4.

During model calibration, this DOS window can be minimized or moved to different location, if it covers the area you want to see.

It should be noted that when specifying boundary fluxes, you should consider mass balance under steady state conditions. If specified boundary fluxes do not follow rule of mass balance, the specification range cannot be approached.

4 DATA PREPARATION AND INPUT INSTRUCTION

4.1 Data Requirement

Data requirement for using MODAC includes two parts. The basic files are the standard MODFLOW input files that should be consistent with the MODFLOW 1996 version. Specific data requirement for parameter estimation using MODAC includes:

- Interpreted potentiometric surface as direct model calibration target, which should be used as initial head for MODFLOW in the BAS file.
- Hydraulic conductivity (or transmissivity) constraints
- Constraints on conductance of head-dependent boundaries, if they are required to be estimated.
- Estimated boundary fluxes as a secondary model calibration target. If information is not available, this can be considered as an optional data requirement, or applied in later stage of model calibration based on professional judgment.

4.2 Input Instructions

4.2.1 Standard MODFLOW Input Files and NFL File

Basic files are standard MODFLOW input files. However, the hydraulic conductivity matrix and Vcont matrix need to be separated from the BCF file, so the values of these matrix can be quickly replaced by the newly estimated values.

You may use a groundwater model GUI to generate standard MODFLOW files first. Then run MODAC to open a NEW...(MODFLOW NAM File). MODAC will generate a NFL file for you and separate the hydraulic conductivity and Vcont matrix from the BCF file.

4.2.2 Interpreted Potentiometric Surface as Direct Target

MODAC uses interpreted potentiometric surface as direct target for hydraulic parameter estimation, although in an entire model calibration process a global calibration target is required as discussed in Section 2.

Requirement for interpreted potentiometric surface includes:

- Interpreted potentiometric surface should honor observed points
- Interpreted potentiometric surface should cover an entire active model domain
- Interpreted potentiometric surface should not be conflict with specified model boundary conditions, e.g., a no-flow boundary should be perpendicular to equal-potential line
- Potentiometric surface is better to be interpreted by hydrogeologist based on hydrogeologic understanding but not simply by contour software

Interpreted potentiometric surface for an entire model domain should be read as the initial conditions for MODFLOW (in a MODFLOW BAS file or attached to a BAS file) for the layer which hydraulic conductivity distribution needs to be calibrated. Input of initial conditions can be directly prepared as matrix or prepared by a GUI. However, caution should be taken to check if the specified initial conditions are reserved on prescribed head boundaries in the ASCII MODFLOW BAS input file.

4.2.3 MAC File

The only additional input file required by MODAC is a MAC file, which contains specifications for parameters used in parameter estimation and various constraints. The MAC file can be created and modified on screen, or prepared by a groundwater model GUI prior to starting MODAC. This MAC file should be included in the NFL file as

DATA 96 XXXXXXXXX.MAC

When using MODAC to generate a NFL file, the above line is included automatically.

Explanation of MAC File Parameters

The parameters as shown in the following MODAC MAC Setup window are explained as follows.

Selecting Parameters for Calibration

The parameters that you can use MODAC to estimate include:

- **Hydraulic conductivity**
- **General head conductance**
- **River conductance**
- **Drain conductance**
- Storage coefficient (not applicable yet)

You may choose appropriate parameter(s) according to your problem.

Selecting Method

Three parameter adjustment methods are included in the MODAC package for estimation of hydraulic conductivity:

- **Gradient** - hydraulic gradient comparison method
- **Head** - hydraulic head comparison method
- **Combined** - hybrid of gradient and head comparison methods

In general conditions, the gradient method is the most powerful one. However, the gradient method alone has some limitation. When boundary conditions are complicated, or constraints on K in certain area have limited a good match of hydraulic head in that area, gradient method may not be flexible enough to allow match of the heads in the rest of area. In this case, combined method or head method could be used alternatively either as the primary method or the secondary method.

Alternating Interval

The *alternating interval* is the number of steps using primary method. If the alternating interval equals 1, adjustment will use one step for primary method and one step for secondary method. If the alternating interval is equal to or greater than 2, adjustment will use two or more steps for primary method and one step for secondary method.

The image shows the 'MODAC MAC SETUP' dialog box. It is divided into several sections for configuring the calibration process.

- Selecting Parameter for Calibration:**
 - ☒ Hydraulic Conductivity or Transmissivity
 - ☒ General Head Conductance
 - ☐ Drain Conductance
 - ☒ River Conductance
 - ☐ Storage Coefficient
- Selecting Method:**

Primary Method	Secondary Method	Alternating Interval
Combined	Combined	1
Head	Head	
Gradient	Gradient	
- Layer Match:** Calibration of Layer 1 for Heads Match in Layer < 1 >
- Parameter Adjustment Step Size:**
 - Step Size: 0.020
 - Maximum Step Size: 0.10
- Smooth Factor:**
 - Upper Ratio (>=1.0): 1.15
 - Lower Ratio (<=1.0): 0.85
- Vertical Anisotropy Ratio of Kh/Kv:**
 - Minimum Vcont Value: 0.0000001
 - Select Layer:
 - Layer 1 Use File <LAYER-01.VRT>
 - Layer 2 Uniform Value 100
- Upper Limits of K:**
 - Select Layer:
 - Layer 1 Use File <LAYER-01.UPL>
 - Layer 2 Uniform Value 100
- Lower Limits of K:**
 - Select Layer:
 - Layer 1 Uniform Value 0.0001
 - Layer 2 Uniform Value 0.009
- Residual criteria for screen plot:** 1.0
- Buttons:** Save MAC, Cancel

Layer Match

Layer Match = 0, no calibration for this layer

Layer Match = Layer number, parameter estimation will directly match the head information of this layer. Case 2 selected this option for all three layers.

Layer Match > 0 and = Other layer number, parameter estimation of the layer will support matching the head information of the other layer. This option is often selected when the layer is hydraulically connected with the other layer that has potentiometric surface while the data in the layer itself are not adequate to generate a representative potentiometric surface. This option was designed considering that potentiometric surface may only be available for uppermost layer in most practical problems. In Case 2, this option can be chosen for layer 2 and layer 3 because the three layers are hydraulically connected. Users are encouraged to try this option. You will see the calibrated results of choosing this option are somewhat close to the results of choosing all layers matching their potentiometric surfaces.

When using MODAC to set or modify ***Layer Match***, you can double click and specify according to your need.

Parameter Adjustment Step Size

Step Size – Step size is the value of scaling factor α used to determine the step size of parameter adjustment as shown in Equation (10) in Appendix A. The greater the step size the faster the change of parameter value. Adjustment of the step size is problem dependent and needs to be cautious.

Maximum Step Size – Maximum value of step size, which limits big change of parameter value that may cause unstable solution.

Smooth Factor

Smooth factor is used to control spatial variation of parameter values. At the early stage you may or may not turn on this function. In the later stage, it is encouraged to turn on this function to force a smooth spatial variation of parameters. The use of smooth factor is problem dependent. Users are encouraged to try under different conditions.

Upper Ratio

Upper smooth factor is used to control the ratio of hydraulic conductivity values in neighboring cells. The value should be greater than or equal to 1.0. The smaller the value the smoother the K distribution. The value can be changed during MODAC operation in the Model Run Dialog window. When both upper and lower smooth factors are equal to 1.0, the smooth effect is maximized.

Lower Ratio

Lower smooth factor is also used to control the ratio of the hydraulic conductivity values in neighboring cells. The value should be greater than 0.0 and less than or equal to 1.0. The greater the value, the smoother the K distribution. The value can be changed during MODAC operation in the Model Run Dialog window. When both upper and lower smooth factors are equal to 1.0, the smooth effect is maximized.

Smooth factors work within each specified zone of constraint on hydraulic conductivity. Smooth will not happen across the boundary of different zones of K constraints.

Vertical Anisotropy Ratio of K_h/K_v

The vertical anisotropy ratio is used in calculation of vertical conductance between layers. Vertical anisotropy ratio of K_h/K_v can be set as a constant for each layer or distributed values using a matrix file. The matrix file can be generated using groundwater model GUI with specified format or free format.

When using MODAC to set or modify the vertical anisotropy ratio, you may double click the layer, then you will see a dialog window as follows:

Set up Vertical Ratio of Layer 1

Select Method

☒ Use uniform Value

☐ Input a matrix file and modify Multiplier

☐ Modify initial Kvalue as constraints

Export property to matrix file

Width of each numeric field

Precision of each field

☒ Field format - Exponential [e]

☐ Field fromat - Fixed [f]

Save Cancel

You have two choices:

- Input a uniform value
- Input an existing matrix file, if you need to, you can modify it

Upper Limits of K

Upper limits of hydraulic conductivity can be set as a constant for each layer or distributed using a matrix file. The matrix file can be generated using groundwater model GUI with specified format or free format. In practical problems, it is important to set constraints on hydraulic conductivity based on field aquifer test results or other supporting data. The uncertainty associated with interpretation of potentiometric surface can be somewhat controlled by interpreted aquifer test results if they are representative.

When using MODAC to set upper limits, you may double click the layer under Upper Limits of K. A set up dialog will show as follows:

Set up Upper Limit of Layer2

Select Method

☒ Use uniform Value

☐ Input a matrix file and modify

☐ Modify initial Kvalue as constraints

Multiplier

Export property to matrix file

Width of each numeric field

Precision of each field

☒ Field format - Exponential [e]

☐ Field fromat - Fixed [f]

Save Cancel

You have three choices:

- Use a uniform value
- Input an existing matrix
- Modify initial K value as constraint by using multipliers

You can click on one of these options and follow the sequential prompt to finish your upper limit setup.

Lower Limits of K

Lower limits of hydraulic conductivity can be set as a constant for each layer or distributed using a matrix file. The matrix file can be generated using groundwater model GUI.

Lower limits can be set as same as upper limits if a user does not want the K values to be changed in certain area.

Residual Criteria for Screen Plot

Residual criteria for screen plot on the bottom-right window can be determined by user according to your conditions.

Input Instruction of MAC file in ASCII Format:

GENERAL

- | | | |
|----|--------------------|---|
| A1 | Record:
Format: | <p>Parameters selected for estimation
free format with space delimited</p> <ul style="list-style-type: none">• HYK – hydraulic conductivity• GHB – general head boundary conductance• DRN – drain conductance• RIV – river conductance <p>For GHB, DRN, RIV, if not selected, they will not be estimated.
HYK will always be estimated.</p> |
| A2 | Record:
Format: | <p>HEADNG
A80</p> <ul style="list-style-type: none">• HEADNG = HYK in the current version. |
| A3 | Record:
Format: | <p>MTHD1, MTHD2, NALT
A5, A5, I5</p> <ul style="list-style-type: none">• MTHD1 – primary method• MTHD2 – secondary method• NALT – number of alternating iterations using primary or secondary method, e.g.,<ul style="list-style-type: none">o If NALT= 2, MODAC uses the primary method for 2 iterations and the secondary method for 1 iteration;o If NALT = 3, MODAC uses the primary method for 3 iterations and secondary method for 1 iteration. |

		• COMB – combined method of gradient comparison and head comparison • GRAD – hydraulic gradient comparison method • HEAD – hydraulic head comparison method
A4	Array: Format:	Layer Match (NLAY) 40I2 • Layer Match is a 1D integer array with double indications: (1) specifying whether the hydraulic conductivity of the layer needs to be calibrated; and (2) if the K values of the layer need to be calibrated, specifying which target will be used for calibration. The position of Layer Match in the array corresponds to sequence of model layers. • Layer Match = 0 – No calibration for the layer • Layer Match $\neq$ 0 – Horizontal hydraulic conductivity of this layer needs to be estimated • Layer Match = Layer sequential number – The potentiometric surface of this layer will be used as a direct target in parameter estimation. • Layer Match = Other layer number – The potentiometric surface of the other layer will be used as indirect target. The hydraulic conductivity of this layer will be estimated to support the other layer in matching the corresponding target.
A5	Array: Reader:	Step Size (NLAY) U1DREL • Step Size is a 1D real array defining the step size, α, for parameter adjustment (Appendix A). Each value in the array corresponds to one model layer. Step size is generally less than 0.1, usually varies between 0.001 to 0.01.
A6	Array: Reader:	Maximum Step Size (NLAY) U1DREL • Maximum Step Size is the maximum value of α. Each value in the array corresponds to one model layer.
A7	Array: Reader:	Upper Smooth Factor (NLAY) U1DREL • Upper smooth factor is used to control the ratio of the hydraulic conductivity values in neighboring cells. The value should be greater than or equal to 1.0. The value can be changed during MODAC operation in the Model Run Dialog window. When both upper and lower smooth factors are equal to 1.0, the smooth effect is maximized.

A8 Array: Lower Smooth Factor
 Reader: U1DREL

- Lower smooth factor is also used to control the ratio of the hydraulic conductivity values in neighboring cells. The value should be greater than 0.0 and less than or equal to 1.0. The smaller the value, the less the smooth effect. The value can be changed during MODAC operation in the Model Run Dialog window. When both upper and lower smooth factors are equal to 1.0, the smooth effect is maximized. Each value in the array corresponding to one model layer.

(Enter A9 only if there is more than one layer in model)

A9 Array: Lower limit of vertical conductance (NLAY-1)
 Reader: U1DREL

- Lower limit of vertical conductance is set to prevent calculated Vcont approach to zero. The default value for the lower limit of vertical conductance is 0.000001.

FOR EVERY LAYER SEQUENTIALLY

(Enter A10 only if there is more than one layer in model)

A10 Record: INCODE, Vertical anisotropy ratio, Coefficient, Form

- If vertical anisotropy ratio is a constant for a layer:
 - INCODE = 0
 - Vertical anisotropy = K_x/K_z
 - Format: I10, F10.2
- If vertical anisotropy ratio is an array for a layer:
 - INCODE = "OPEN/CLOSE"
 - Vertical anisotropy ratio = file name of the array
 - Coefficient
 - Form: Format of the array
 - Format: Free format

A11 Record: INCODE, Upper limit of K for the layer, Coefficient, Form

- IF upper limit is a constant for a layer:
 - INCODE = 0
 - Upper limit = constant
 - Format: I10, F10.2
- IF upper limit is an array for a layer
 - INCODE="OPEN/CLOSE"
 - Upper limit = file name of the array
 - Coefficient
 - Form: Format of the array
 - Format: Free format

A12 Record: INCODE, Lower limit of K for the layer, Coefficient, Form

- IF lower limit is a constant for a layer
 - INCODE = 0
 - Lower limit = constant
 - Format: I10, F10.2
- IF lower limit is an array for a layer
 - INCODE="OPEN/CLOSE"
 - Lower limit = file name of the array
 - Coefficient
 - Form: Format of the array
 - Format: Free format

GENERAL

A13 Record: Head residual criteria for screen plot
Format: F10.2

For illustration purpose, an example is provided as follows.

EXAMPLE 1

HYK RIV	<i>hydraulic conductivity and river conductance are estimated</i>		
HYK			
COMB HEAD 1	<i>Primary - combined, secondary – head, Nalt = 1</i>		
1 1 1	<i>All layers require K estimation; Layers 2 and 3 support layer 1</i>		
96 1.0 (10f12.4)	0		
5.0000e-03 5.0000e-03 5.0000e-03		<i>step size for each layer</i>	
96 1.0 (10f12.4)	0		
2.0000e-02 2.0000e-02 2.0000e-02		<i>Maximum step size for each layer</i>	
96 1.0 (10f12.4)	0		
1.1500e+00 1.1000e+00 1.1000e+00		<i>Upper smooth factor for each layer</i>	
96 1.0 (10f12.4)	0		
8.5000e-01 9.5000e-01 9.5000e-01		<i>Lower smooth factor for each layer</i>	
96 1.0 (10f12.4)	0		
1.0000e-08 1.0000e-08		<i>Lower limit for vertical conductance</i>	
OPEN/CLOSE layer1.vrt 1.0 (FREE) -1		<i>Vertical Ratio for Layer 1</i>	
OPEN/CLOSE LAYER-01.UPL 1.0 (FREE) -1		<i>Upper Limit of Layer1</i>	
01.0000e-01	0	<i>Lower limit of Layer 1</i>	
OPEN/CLOSE layer2.vrt 1.0 (FREE) -1		<i>Vertical Ratio for Layer 2</i>	
0 1000.000	0	<i>Upper limit of Layer 2</i>	
01.0000e-01	0	<i>Lower limit of Layer 2</i>	
OPEN/CLOSE layer3.vrt 1.0 (FREE) -1		<i>Vertical Ratio for Layer 3</i>	
0 1000.000	0	<i>Upper limit of Layer 3</i>	
01.0000e-01	0	<i>Lower limit of Layer 3</i>	
1.00		<i>Head residual criteria for screen plot</i>	

4.2.4 Constraints

Constraints on hydraulic parameters for most of real-world problems are necessary. Constraints on hydraulic conductivity (transmissivity) and conductance of head-dependent boundary are in two different formats.

4.2.4.1 Constraints on Hydraulic Conductivity (or Transmissivity)

Upper and lower constraints on hydraulic conductivity (transmissivity) can be specified as constant for an entire model domain for each layer, or as distributed values using array with the concept of zonation.

Zonation of upper and lower constraints can be generated using GUI and be modified in MODAC during model calibration. Format of distributed constraints should be consistent with user's specification in MAC file.

If the constraints are set as zones, the smooth function will be applied within each zone, but not across boundary between zones. *Zone Average* also applies within each zone following the zones specified for constraints.

4.2.4.2 Constraints on Conductance of Head-Dependent Boundary

Constraints on conductance for head-dependent boundary conditions, such as River, General Head, and Drain, are set within MODFLOW input files for the corresponding head-dependent boundaries. In each of these head-dependent boundary input files, an auxiliary parameter specified as [xyz] can be used to specify upper and lower limits for each conductance corresponding to each model cell.

If user did not specify upper and lower limits on conductance, for user's convenience, MODAC sets the default upper and lower limits automatically for user. The format follows the standard MODFLOW (1996) input files for any head-dependent boundary input files. The default upper limit is four times of your specified conductance, and the default lower limit is one-fourth of your specified conductance. The following is an example of a river input file with specified upper and lower limits.

Example – River Package Input file with specified constraints

8	51	AUX CLW	AUX CUP				
8							
1	9	12	6139.040	134.17	6138.54	20.00	2000.00
1	9	13	6140.710	20.00	6140.21	20.00	2000.00
1	9	14	6140.500	20.00	6140.00	20.00	2000.00
1	9	15	6140.860	20.00	6140.36	20.00	2000.00
1	9	21	6139.350	10.00	6138.85	10.00	1000.00
1	9	22	6138.950	27.01	6138.45	10.00	1000.00
1	9	23	6137.370	135.44	6136.87	10.00	1000.00
1	9	24	6137.350	73.53	6136.85	10.00	1000.00

4.2.5 Flux Targets on Boundary

Two types of flux targets can be used in model calibration. One is total flux through one given boundary condition, and the other is distributed flux at individual model cells. For total flux, either total inflow or total outflow should be specified, but not the net flux of the sum of inflow and outflow. A range of estimated flux rates as upper limit and lower limit can be specified or reviewed within the MODAC dialog window (page 19-20). A negative sign means aquifer loses water to boundary while a positive sign means aquifer gains water from boundary.

The range of total fluxes for the GHB, River, Drain boundaries are written in the second line of each corresponding input files. You may review or modify them in the ASCII input files (see example as follows) too.

Example – River Package Input file with specified constraints and flux targets

	686	50	AUX	CLW	AUX	CUP	AUX	FLW	AUX	FUP
	686	-7.80E+04	-8.50E+04							
1	142	192	89.040	82.17	88.54	55.80	893.00	0.01	120.00	
1	142	191	89.500	521.46	89.00	243.00	3890.00	0.01	120.00	
1	142	190	89.300	237.83	88.80	162.00	2590.00	0.01	120.00	

In this example,

AUX CLW – Lower limit for conductance

AUX CUP – Upper limit for conductance

AUX FLW – Lower limit for target flux

AUX FUP – Upper limit for target flux

In second line, -7.80E+04 and -8.50E+04 are specified lower limit and upper limit of total flux out of all river boundary cells.

In each model cell, the values in the very last two columns are specified flux targets, and the values in the two columns second to the last two columns are specified constraints on conductance.

Note, after modifying these files, be sure to save them in the format as .csv file in Microsoft Excel. When browsing the file in the MODAC dialog window, searching for the corresponding .csv file.

The estimated range of flux for constant head boundary is specified in the CHD file.

4.2.6 Observed Data File

Observed hydraulic heads at monitoring wells can be input directly during MODAC calibration. This data file should be located in the same folder used for calibration. The name of the file should be: **Target.dat**. The format of the file can be free or formatted, but should follow the sequence as follows:

Head line

Well-name	X-coordinate	Y-coordinate	Water-level	Layer
-----------	--------------	--------------	-------------	-------

An example is provided as follows.

Name,X,Y,Water-level,Layer
Well-1,4659.1,6662.7,62.16,1
Well-2,4592.2,6776.4,61.81,1
Well-3,8307.6,10455.2,122.57,1
Well-4,7847.5,10262.8,117.36,1
Well-5,7237.1,10001.6,107.02,1
Well-6,7248.1,10006.2,106.94,3
Well-7,7242.2,10005,106.94,2

4.2.7 Culture Lines

MODAC also prepares a culture lines file for user with a name as CULTURE.BLN. If your site coordinates are different from the model coordinates, you need to provide the X and Y site coordinates for your model origin (offset).

You may also introduce background culture lines with the standard format of the SURFER BLN file in this file.

APPENDIX A – THE INVERSE METHOD

MODAC is a package that includes two parts: MODFLOW and the inverse methods that perform parameter adjustment. There are three inverse methods used in the package. The primary inverse method is the hydraulic gradient comparison method (Guo and Zhang 1994, Guo and Zhang 2000). The other two methods are the hydraulic head comparison method and the combined methods (hybrid of hydraulic gradient and hydraulic head comparison methods). These two methods are approximation of the hydraulic gradient comparison method. The inverse methods can be used independently with any groundwater flow model package, either based on finite difference method or finite element method. MODAC couples these methods with MODFLOW for user's convenience. To introduce the concept of the inverse method, here we only discuss the hydraulic gradient comparison method.

The hydraulic gradient comparison method is an inverse method for estimation of aquifer hydraulic conductivity (or transmissivity) and head-dependent boundary conductance for a groundwater flow model under steady state conditions or transient conditions. This method, following formal optimization techniques, defines its objective function to minimize differences between interpreted (observed) and simulated hydraulic gradients, which leads to minimization of differences between observed and simulated hydraulic heads without additional specification of boundary conditions.

There are two key features in this method. The first one is that the derived optimality conditions have an explicit form with a clear hydrogeology concept that is consistent with Darcy's law. The second one is that the derived optimality conditions are spatially independent, as they are a function of only local hydraulic conductivity and local hydraulic gradient; therefore a multi-dimensional optimization problem can be solved by many one-dimensional optimization procedures simultaneously, which results in substantial reduction of computation time. No preconceived zonation of parameter is required; estimation of hydraulic conductivity distribution is performed on a cell-by-cell basis.

A brief summary of the hydraulic gradient comparison method and the numerical procedure are presented in the following sections.

Objective Function

Conventionally, the governing equation for groundwater flow in a heterogeneous, confined aquifer under steady state conditions is defined as:

$$\nabla \cdot (T \cdot \nabla h) = q \quad \text{in } R \quad (1)$$

subject to the boundary conditions

$$h = h_1 \quad \text{on } B_1 \quad (2a)$$

$$-T \cdot \nabla h \cdot n = q_1 \quad \text{on } B_2 \quad (2b)$$

$$-T \cdot \nabla h \cdot n = \tau(h^* - h) \quad \text{on } B_3 \quad (2c)$$

where

∇	gradient operator
T	transmissivity tensor
h	hydraulic head
q	source-sink term
R	flow domain
B_1	boundary of domain R for prescribed head condition
B_2	boundary of domain R for prescribed flux condition
B_3	boundary of domain R for head-dependent condition
n	unit vector normal to boundary
h_1	prescribed head at prescribed head boundary
q_1	prescribed flux at prescribed flux boundary
h^*	prescribed head at a general head boundary
τ	conductance of the general head boundary

From the literature, the common approach to identification of distributed hydraulic parameters (e.g., transmissivity) is to define an objective function (OBJ) that minimizes the differences between observed and simulated hydraulic heads (h^o and h). If a classical least square error criterion is used, the objective function to be minimized is

$$OBJ = \sum_{i=1}^{N^o} (h - h^o)_i^2 \quad (3)$$

where N^o is the total number of hydraulic head observations. This is often used as the general performance criteria in inverse models to describe “how good” that fit head observations. Equation (3) is a typical multi-dimensional optimization problem, which is often solved using the Gauss-Newton algorithm [Cooley 1977, 1979]. Several currently available automated calibration computer codes, including MODINV [Doherty, 1990], MODFLOWP [Hill, 1991], and PEST [Doherty, 1994] were developed based on this nonlinear least-squares regression approach.

Like the conventional approach to the inverse problem described earlier, the hydraulic gradient comparison method for parameter estimation is also formulated as a mathematical optimization problem. However, the objective function is defined differently than in Equation (3). In this method the objective function is to minimize the differences between simulated and interpreted (observed) hydraulic gradients, as shown in Equation (4), rather than to minimize the differences between observed and simulated hydraulic heads. The objective function for the hydraulic gradient comparison method is defined as:

$$OBJ = \int_R (\nabla h - \nabla h^o) \cdot (\nabla h - \nabla h^o) dx dy \quad (4)$$

where ∇h and ∇h^o are simulated and interpreted (observed) hydraulic gradients. In Equation (4), minimization of hydraulic gradient differences under given boundary conditions is equivalent to minimization of hydraulic head differences using Equation (3). As we know, the governing equation for groundwater flow is a second order partial differential equation in hydraulic head that, when solved, yields a unique hydraulic head distribution for a given set of boundary conditions that should satisfy a well-posed problem in partial differential equations [DuChateau and Zachmann 1989]. Simply stated, a well-posed problem requires that flux boundary conditions should not be specified for all boundaries. Similarly, if the first order partial differential equation in hydraulic head is given, which defines the hydraulic gradient of a flow field, the head distribution is also unique given the same set of boundary conditions as for the governing equation. Therefore, minimization of hydraulic gradient differences can achieve the same results as minimization of head differences. In summary, this method does not require additional specification of boundary condition other than the well-posed problem defined by the governing equation.

When the boundary conductance for head-dependent type boundary needs to be estimated at the same time when hydraulic conductivity is estimated, the objective function of Equation (4) is expanded as:

$$OBJ = \int_R (\nabla h - \nabla h^o) \cdot (\nabla h - \nabla h^o) dx dy + \int_{B_3} (h - h^o)^2 ds \quad (5)$$

Optimality Conditions

Based on the objective function (Equation (5)), the optimality condition was derived (Guo and Zhang 2000) using the constrained calculus of variations method [Morel-Seytoux and Guo, 1990] as follows:

$$\frac{\partial L}{\partial T_j} = -\frac{2}{T_j} \int_{r_j} (\nabla h_j - \nabla h_j^o) \cdot \nabla h_j \, dx dy \quad j = 1, 2, \dots, N \quad (6)$$

Equation (6) can be considered as the optimality condition for parameter T_j when it approaches zero.

Similarly, the partial derivative of the objective function with respect to τ_l can be obtained,

$$\frac{\partial L}{\partial \tau_l} = \frac{2}{\tau_l} \int_{b_l} (h_l^* - h_l) (h_l - h_l^o) \, ds \quad l = 1, 2, \dots, M \quad (7)$$

When Equation (7) approaches zero, it approaches the optimality condition.

For an unconfined aquifer, the optimality conditions for hydraulic conductivity K_j can be derived by simple substitution. The resulting optimality conditions for an unconfined aquifer are:

$$\frac{\partial L}{\partial K_j} = -\frac{1}{2K_j} \int_{r_j} [\nabla h_j^2 - \nabla(h_j^o)^2] \cdot \nabla h_j^2 dx dy \quad j = 1, 2 \dots N \quad (8)$$

$$\frac{\partial L}{\partial \tau_l} = \frac{1}{2\tau_l} \int_{b_l} (h_l^{*2} - h_l^2)(h_l^2 - h_l^{o2}) ds \quad l = 1, 2 \dots M \quad (9)$$

Hydrology Concept in the Optimality Conditions

An important feature implied in Equation (6) is that the optimality condition is consistent with Darcy's law. From mathematical point of view, to make the partial derivative $\partial L / \partial T_j$ approach the optimality condition, according to Equation (6), if $(\nabla h - \nabla h^o) \cdot \nabla h > 0$, the value of transmissivity (T) needs to be increased. Conversely, if $(\nabla h - \nabla h^o) \cdot \nabla h < 0$, the value of T for the partial derivative must be decreased to approach the optimality condition. This concept is consistent with Darcy's law.

Spatial Independence of Optimality Conditions

Another important feature that is implied in Equation (6) is the spatial independence of the optimality conditions. The partial derivative of the objective function with respect to transmissivity is solely a function of local hydraulic conductivity and local hydraulic gradient. It is not related to hydraulic conductivity or hydraulic gradient at other locations. In other words, under steady state conditions, adjustment of a hydraulic parameter, using the hydraulic gradient comparison method, is spatially independent of adjustment of that parameter at other locations. Equation (7) implies the similar feature.

Because of the spatial independence of the optimality conditions, a multi-dimensional optimization problem can be solved by many one-dimensional optimization procedures. As stated by Yeh [1986], because of the spatial dependence of hydraulic head on distributed hydraulic parameters, an inverse problem is usually formulated as a multi-dimensional optimization problem, which requires solution of a system of equations simultaneously. When the number of parameters increases, the computational time increases exponentially. In contrast to the traditional inverse technique, the spatial independence of the optimality conditions for the hydraulic gradient comparison method allows a multi-dimensional optimization problem to be solved by many one-dimensional optimization procedures simultaneously. Therefore, the solution procedures based on the hydraulic gradient comparison method are much simpler, and the dimension of the estimated parameters is not limited. This is one of the major reasons that the hydraulic gradient comparison method can

be easily applied to field projects, while the traditional inverse technique encounters difficulty when it is applied to complex real-world problems.

Numerical Procedure

The numerical procedure to implement the hydraulic gradient comparison method is an iterative process. The procedure starts from a set of initial estimates of hydraulic conductivity values. At each iteration, a model simulation is performed, then hydraulic conductivity values at each model cell are adjusted simultaneously based on Equations (8) and (9) for unconfined conditions, or Equations (6) and (7) for confined conditions. The adjustment of hydraulic conductivity follows the following gradient search method

$$K_i^{j+1} = K_i^j - \alpha \left(\frac{\partial L}{\partial K_i} \right)^j \quad i = 1, 2, \dots, N \quad (10)$$

subject to:

$$K_{\min,i} < K_i < K_{\max,i}$$

and

$$\tau_l^{j+1} = \tau_l^j - \beta \left(\frac{\partial L}{\partial \tau_l} \right)^j \quad l = 1, 2, \dots, M \quad (11)$$

subject to:

$$\tau_{\min,l} < \tau_l < \tau_{\max,l}$$

where

K	hydraulic conductivity
τ	conductance of the head-dependent boundary
i	cell index,
l	boundary section index for boundary B ₃
j	iteration index
$\partial L / \partial K_i$	partial derivative of the objective function with respect to the hydraulic conductivity at cell i
$\partial L / \partial \tau_l$	partial derivative of the objective function with respect to the conductance at section l

The values of $\partial L / \partial K$ and $\partial L / \partial \tau$ are calculated using Equations (8) and (9), or (6) and (7). Coefficients α and β are scaling factors to determine the step size of parameter adjustment.

This numerical procedure has been implemented to MODAC, a computer code that performs an iterative procedure of the USGS MODFLOW [McDonald and Harbaugh, 1988; Harbaugh and McDonald, 1996] simulation and hydraulic parameter adjustment as described above. In an iterative process, about 95 percent or more computer time is used by MODFLOW simulation, and only 5 percent or less is used for parameter adjustment.

Smooth Technique

In the numerical procedure, a smoothing technique is implemented within prior specified constraints on hydraulic parameters. The minimization of hydraulic gradient differences is performed simultaneously with a minimization of spatial variation of parameter values. Thus, estimated hydraulic parameters can vary smoothly within each zone to reflect the continuity and heterogeneity of the geologic properties; potential over parameterization is controlled.

APPENDIX B – DISSCUTION OF HYPOTHETICAL CASE 1

In order to show how MODAC works, hypothetical case 1 and the associated electronic files are included for discussion and screen demonstration. This section discusses:

- Purpose of the hypothetical case study
- How the hypothetical case was generated
- How to understand the process of parameter estimation of the hypothetical case
- What the results of hypothetical case indicate

Purpose of Hypothetical Case Study

The original purpose of the hypothetical case study was to test the numerical performance of the hydraulic gradient comparison method (Guo and Zhang 2000). The specific purpose of including the case study in this package is to discuss the concept via an example and to provide an on-line demonstration for users to understand the MODAC working process.

Development of Hypothetical Case

The hypothetical case assumes an unconfined and heterogeneous groundwater flow system. The specified hydraulic conductivity distribution ranges from 0.03 m/day to 3.05 m/day (0.1 ft/day to 10.0 ft/day), as shown in Figure 1(a). The bottom elevation of the aquifer is variable. A one-layer, finite difference grid consisting of 100 rows and 100 columns with a uniform cell dimension of 30.5 m (100 ft) by 30.5 m (100 ft) is superimposed on the flow system. Boundary conditions consist of general head boundary, prescribed flux, and no-flow. The conductance of the general head boundary is constant and specified as 23.2 m²/day (250 ft²/day). Several source/sink terms exist within the model domain, including two pumping wells, two injection wells, and areal positive and negative ground water recharge. The hydraulic head distribution (solid line in Figure 2) was generated using MODFLOW input file data under steady-state condition.

Parameter Estimation Processes

In the parameter estimation process, the hydraulic conductivity distribution and general head boundary conductance are assumed unknown. The generated hydraulic head distribution in Figure 2 was assumed to be the “interpreted” potentiometric surface and is used as the calibration target for parameter estimation. In total, 10,000 hydraulic conductivity values and 100 river conductance values need to be estimated given 10,000 known hydraulic head values, specified boundary conditions, and other parameters.

Parameter estimation is an iterative forward process, which follows the numerical procedure as described in Section 2. The initial hydraulic conductivity distribution is assumed to be constant over the entire model domain. The initial RMSE-map can be as high as about 6 feet or more, while after a number of iterations of alternating model simulation and parameter adjustment, the RMSE-map could reach a level lower than 0.1 feet, depending on

number of calibration steps, method selected, and/or smooth factor chosen. Eventually, the simulated hydraulic head contours (red color) will closely match the target contours (blue color) in all areas, and residuals will disappear from the right-bottom window. Because there is no uncertainty associated with model boundary conditions, potentiometric surface, and other parameters, the simulated head contours can perfectly match the observed head in theory.

This RMSE-map, defined as the root mean squared error of head (RMSEH), is the average of the squared differences in simulated and “interpreted” heads. For the purpose of testing the numerical procedure, we also calculated the average of the squared differences in simulated and “interpreted” hydraulic gradients, referred to as the root mean squared error of gradient (RMSEG). Comparison of RMSEH and RMSEG is displayed in Figure 3. Both error curves have the same trend, which demonstrates that minimizing the differences in hydraulic gradients has the same effect as minimizing the differences in hydraulic heads.

One important goal of the hypothetical case study was to test if the estimated hydraulic conductivity distribution can approach the true values of the specified hydraulic conductivity field and hydraulic conductance of the boundary. The criterion for the test was specified as the average relative percent error of K (MRPEK), calculated as:

$$MRPEK = \sqrt{\frac{1}{n} \sum_1^n \left[\frac{(K_e - K_t)}{K_t} \times 100\% \right]^2} \quad (1)$$

where

K_e	estimated hydraulic conductivity
K_t	true hydraulic conductivity
n	total number of parameters

The estimated K distribution (Figure 1(b)) is plotted in comparison to the specified K distribution in Figure 1(a), which shows the difference between the estimated and specified K distributions is minimal. The estimated boundary conductance, ranging from 21 m²/day to 25.9 m²/day and with a mean of 23.3 m²/day, is also close to the specified conductance of 23.2 m²/day.

Parameter estimation was conducted four times using different initial values of uniform K, which are 0.3 m/day, 0.9 m/day, 1.8 m/day, and 2.7 m/day, respectively, and an initial conductance of 3.6 m²/day. The initial MRPEK was as high as 1600 percent. During the estimation processes, values of MRPEK were smoothly reduced to less than 7 percent (Figure 4) after 40 iterations for all cases using different initial values of K.

Indication of Hypothetical Case Results

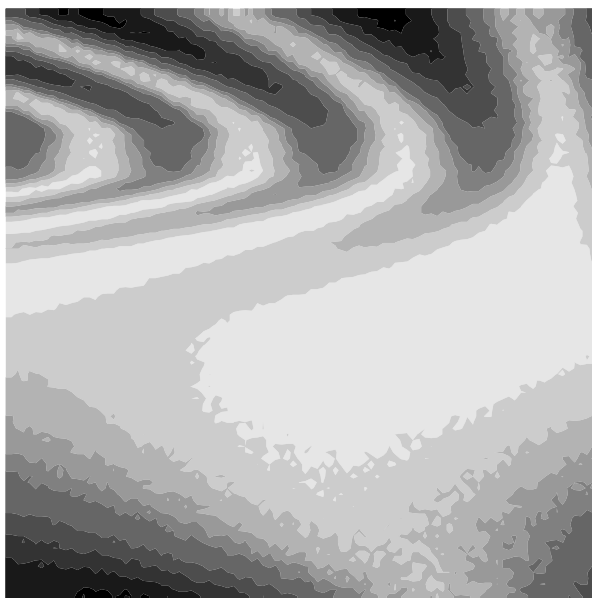
The hypothetical case study results indicate that the hydraulic gradient comparison method is correct mathematically. Simultaneously solving many one-dimensional optimization

problems over an entire model domain can lead to minimization of the differences between simulated and interpreted hydraulic gradients and heads over the entire model domain. In other words, if the optimality condition at every model cell is approached, the objective function for the entire model domain is approached.

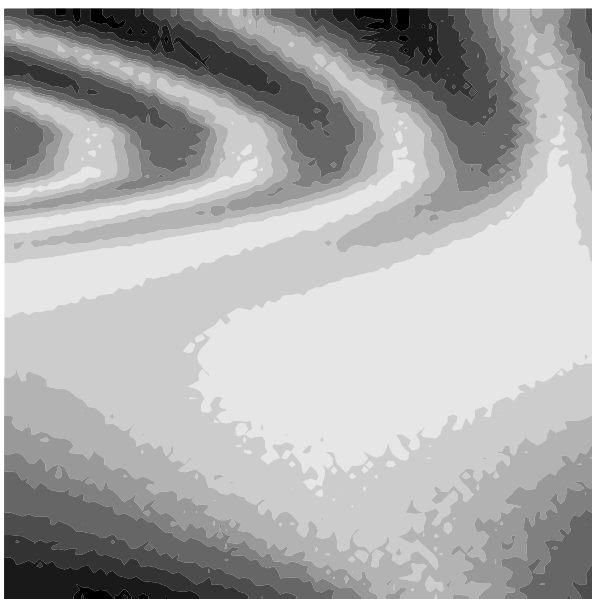
The results of the hypothetical case study also indicate that

- (1) Where the hydrogeologic conditions are completely known (i.e., the problem is not ill-posed), it is mathematically possible to estimate hydraulic conductivity and conductance to a level that is close to “true” values;
- (2) Using different initial values of K , the method can lead to same parameter estimation results.

However, it should be noted in a practical problem, because we cannot avoid uncertainty in conceptual model development, boundary conditions, and hydrologic parameters, estimation of hydraulic parameters cannot avoid certain uncertainty. The only way to reduce such uncertainties is to apply MODAC in an iterative calibration procedure with a global calibration target (Section 2). Successful application of MODAC relies on good conceptual model development.



(a) Generated Hydraulic Conductivity Distribution



(b) Calibrated Hydraulic Conductivity Distribution

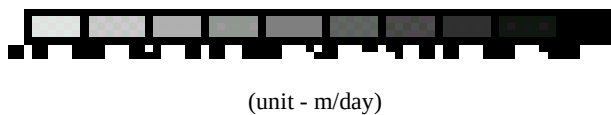


Figure 1. Comparison of specified and estimated hydraulic conductivity distributions

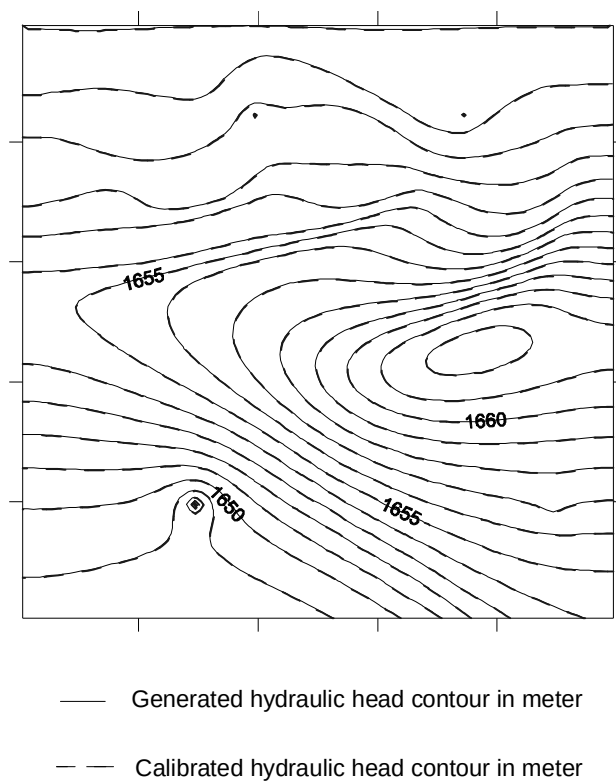


Figure 2. Comparison of generated and calibrated hydraulic head distributions

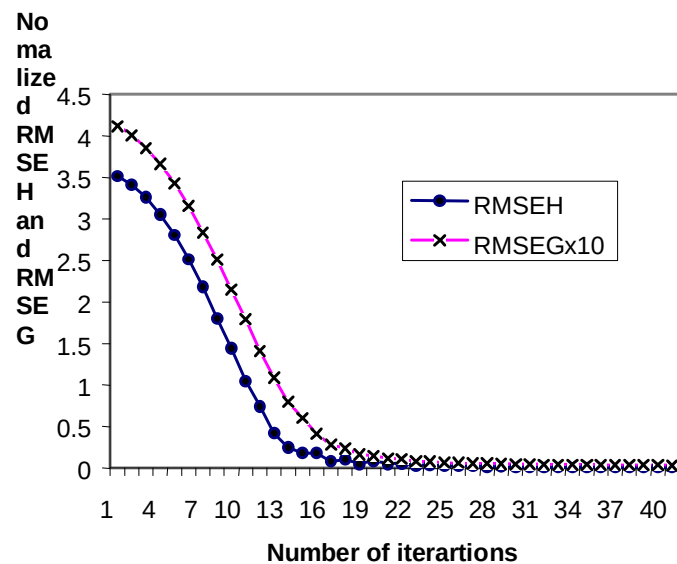


Figure 3. The root mean squared error of head (RMSEH) and the root mean squared error of gradient (RMSEG) versus calibration iterations

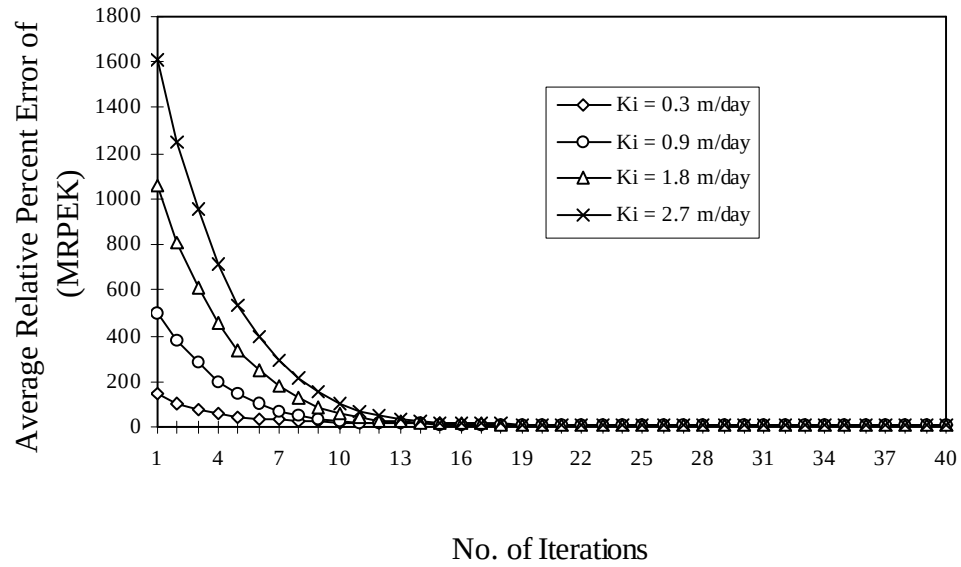


Figure 4. The average relative percent error of hydraulic conductivity (MRPEK) versus calibration iterations using different initial values of hydraulic conductivity

REFERENCES

- Cooley, R. L. 1979. A method of estimating parameters and assessing reliability for models of steady state groundwater flow, 2, Application of statistical analysis. *Water Resources Research* 15, no. 3: 603–617.
- Doherty, J. 1990. MODINV. Australian Center for Tropical Fresh-water Resources, Townsville, Australia. 278 pp.
- Doherty, J. 1994. PEST. Watermark Computing, Corinda, Australia. 122 pp.
- DuChateau, Paul and David Zachmann, 1989. Applied Partial Differential Equations. Harper & Row, Publishers, New York. 620 pages.
- Guo, Xiaoniu and Chuan-Mian Zhang, 1994. Use of the physical feature of groundwater flow system to reduce the mathematical complexity in parameter identification - a practical and efficient automated procedure. In: *Proceeding of the 1994 Groundwater Modeling Conference*, Fort Collins, Colorado, page 111-118, 1994.
- Guo, Xiaoniu and Chuan-Mian Zhang, 2000. Hydraulic gradient comparison method to estimate aquifer hydraulic parameters under steady-state conditions, *Ground Water* 38, No. 6: 815-826.
- Harbaugh, A. W., and M. G. McDonald. 1996. Programmer's documents for MODFLOW-96, an update to the U.S. Geologic Survey modular finite-difference ground-water flow model. USGS Open-File Report 96–486.
- Harbaugh, A. W., E. R., Banta, M. C. Hill, and M. G. McDonald. 2000. MODFLOW-2000, The U.S. Geologic Survey modular ground-water model – user guide to modularization concept and the ground-water flow processes. USGS Open-File Report 00-92.
- Hill, M. C. 1992. A computer program (MODFLOWP) for estimating parameters of a transient, three-dimensional groundwater flow model using nonlinear regression. USGS Open-File Report 91–484.
- McDonald, M. G., and A. W. Harbaugh. 1988. A modular three-dimensional finite-difference groundwater flow model. USGS Open-File Report 83–875.
- Morel-Seytoux, H. J. and Xiaoniu Guo, Application of Constrained Calculus of Variations to the Inverse Problem in Groundwater. Report No. 90.5 Hydrowar Reports Division, *Hydrology Days Publications*, 57 Selby Lane, Atherton, CA 94027, 1990.
- Yeh, W. W.-G., Review of Parameter Identification Procedures in Groundwater Hydrology: Inverse Problem. *Water Resour. Res.*, 22(2), pp. 95-108, 1986.